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OVERVIEW OF THE USE OF ATHENA FOR THERMAL-HYDRAULIC ANALYSIS OF SYSTEMS WITH LEAD-BISMUTH COOLANT

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ABSTRACT

The INEEL and MIT are investigating the suitability of lead-bismuth cooled fast reactors for producing low-cost electricity as well as for actinide burning. This paper is concerned with the general area of thermal-hydraulics of lead-bismuth cooled reactors.

The ATHENA code is being used in the thermal-hydraulic design and analysis of lead-bismuth cooled reactors. The ATHENA code was reviewed to determine its applicability for simulating lead-bismuth cooled reactors. Two modifications were made to the code as a result of this review. Specifically, a correlation to represent heat transfer from rod bundles to a liquid metal and a void correlation based on data taken in a mixture of lead-bismuth and steam were added the code. The paper also summarizes the analytical work that is being performed with the code and plans for future analytical work.

INTRODUCTION

Lead-bismuth is currently being considered as a coolant for a variety of reactors (Buongiorno et al., 1999a; Buongiorno et al., 1999b; Zaki and Sekimoto, 1995; and Greenspan et al., 1998) designed to produce low-cost electricity and/or burn actinides. The economic advantages of lead-bismuth arise from the possibility of developing passively safe reactors with long core lifetimes, possibly in excess of 15 years, combined with lower capital and operating costs. The ability to burn actinides created by the current generation of light water reactors is also an attractive feature of lead-bismuth cooled reactors.

The Idaho National Engineering and Environmental Laboratory (INEEL) and the Massachusetts Institute of Technology (MIT) are jointly investigating the potential of lead-bismuth cooled fast reactors for producing low-cost electricity as well as for actinide burning. The project goal is to identify and analyze key technical issues in core neutronics, thermal-hydraulics, fuels, economics, and materials associated with the development of this reactor concept.

This paper is concerned with the general area of thermal-hydraulics and specifically provides an overview of the modifications to and use of the ATHENA code (Carlson et al., 1986), which is being used in the thermal-hydraulic design of the reactor. The ATHENA code is incorporated as a compile time option in the RELAP5-3Dχ computer code (the RELAP5-3D Development Team, 1999), which in turn is an extension of RELAP5/MOD3 (the RELAP5 Development Team, 1995).

RELAP5 was developed for the thermal-hydraulic analysis of light water reactors and related experimental systems during loss-of-coolant accidents and operational transients. The code originally contained a one-dimensional, nonhomogeneous, and nonequilbirum model for two-phase flow and a point model for reactor kinetics. However, the RELAP5-3Dχ code contains multi-dimensional models for flow and reactor kinetics.

The ATHENA code retains all of the capabilities of RELAP5-3Dχ, but allows the use of working fluids other than water. The code was originally developed to support the Fusion Safety Program, which required a general thermal-hydraulic analysis capability for systems containing other fluids. The code currently can simulate many different fluids, including water, helium, hydrogen, nitrogen, sodium, lithium, and ammonia among others. Liquid, vapor, and two-phase properties are included for each fluid. Lead-bismuth fluid properties were added to ATHENA to support the current investigation of fast reactor designs.

The RELAP5 series of codes has been extensively used and assessed for the thermal-hydraulic analysis of light water reactors. However, the ATHENA code has not been assessed as thoroughly for non-aqueous fluids. Consequently, the applicability of ATHENA for analyzing reactors cooled by lead-bismuth was evaluated. This evaluation determined that the code was generally applicable for such analysis, but also indicated some shortcomings. As a result, two modifications were made to the code to enhance its capability to model lead-bismuth cooled reactors.

The modified ATHENA code has been used to perform and confirm preliminary design calculations. The code has also been used to aid in the design of a corrosion experiment that will be conducted at the INEEL. ATHENA will continue to be used to perform design and confirmatory calculations as the design of the lead-bismuth cooled reactor evolves. The code also will be used to determine the safety margins during several reactor transients.

This paper summarizes the current design of the lead-bismuth cooled reactor, the ATHENA applicability review and code modifications, and the analytical work that has been performed with the code.

NOMENCLATURE

D = diameter (m)
Fr = Froude number
Nu = Nusselt number
P/D = pitch to diameter ratio
Pe = Peclet number
P_{sat} = saturation pressure, Pa
Q_R = volumetric flow ratio
Re = Reynolds number
T = temperature, K
We = Weber number
g = acceleration due to gravity (m/s^2)
j = superficial velocity (m/s)
k = thermal conductivity (W/m-K)
x = flow quality

Greek

α = gas volume fraction
μ = dynamic viscosity (kg/m-s)
σ = surface tension (N/m)
ρ = density (kg/m^3)
ν = kinematic viscosity (m^2/s)

Subscripts

f = liquid
g = gas

REACTOR DESIGN

A preliminary design of a lead-bismuth cooled reactor is illustrated in Fig. 1. The reactor core and heat exchangers are integrated into a pool design. The normal flow path is from the core up through a riser into an upper pool region, then downwards through heat exchangers and a downcomer, and back to the bottom of the core.

Both natural and forced convection designs are currently being considered, the natural convection design at MIT and the forced convection design at INEEL. Forced convection will be obtained either with pumps located in the downcomer or by the injection of an inert gas into the riser. Different options for the fluid on the secondary side of the heat exchangers are also being considered, including water and helium. A conventional steam cycle would be used with water, while a gas turbine cycle would be used with helium. An alternative design will also be evaluated at MIT in which steam will be produced by injecting liquid water directly into the riser, eliminating the need for heat exchangers. Details of these designs are presented elsewhere (Buongiorno et al., 1999a and Buongiorno et al., 1999b).

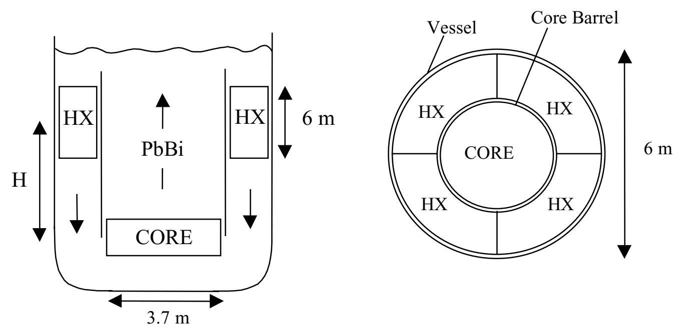

Fig. 1. Preliminary reactor design (from Buongiorno et al., 1999a).

LEAD-BISMUTH FLUID PROPERTIES

Lead-bismuth fluid properties were added to the code since they were considerably different than those for other fluids currently in ATHENA. The equation of state for the lead-bismuth eutectic was developed (Shieh, 1999) in several steps as described below. First, the specific heats for both lead and bismuth up to the melting point of the alloy were obtained from standard tables (Hultgren et al., 1973). The specific heat of the alloy was computed as a weighted average of the lead and bismuth values according to their mass fractions. A simple integration technique was then used to find the enthalpy of the alloy in the solid state up to the melting point. This was then added to latent heat of fusion data to obtain the enthalpy of the liquid alloy at the melting point. The density and temperature at the melting point were also obtained from the tables.

A soft sphere model (Young, 1977) was then used to find the equation of state of the alloy. The soft sphere model is based on the generalized Van der Waal's equation that has five adjustable parameters. Two of these parameters plus two constants used in the model are the same for both lead and bismuth and therefore the same for the alloy. The procedure to find the remaining three parameters is to solve two simultaneous nonlinear equations, i.e.

Pressure at the melting point = 0 (1)

and

Energy at the melting point = enthalpy at melt (2)

These two equations were successfully solved for the three parameters using an iterative procedure. One parameter was fixed and the two equations were solved for the remaining two parameters. The parameter that was fixed was then allowed to vary until an optimal fit was achieved for enthalpy and specific volume at temperatures greater than the melting point. The liquid enthalpy from the resulting model was within 4% of the values derived for the eutectic based on the elemental data of Hultgren et al. (1973) over a wide temperature range as shown in Fig. 2. The liquid specific volume from the model was within 1% of the data of Kutateladze et al. (1970) over a wide temperature range as shown in Fig. 3.

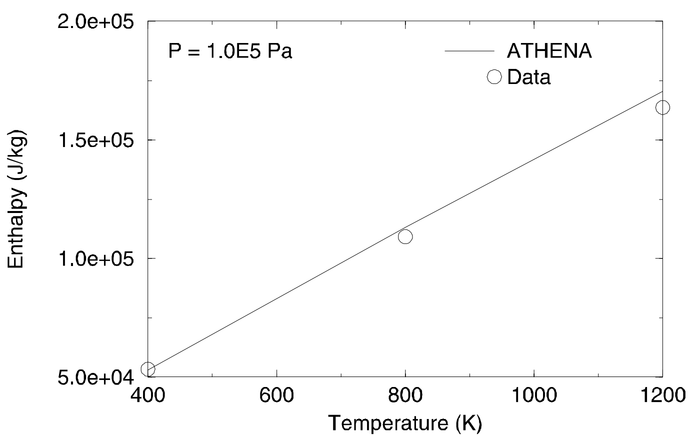

Fig. 2. Enthalpy of liquid lead-bismuth versus temperature.

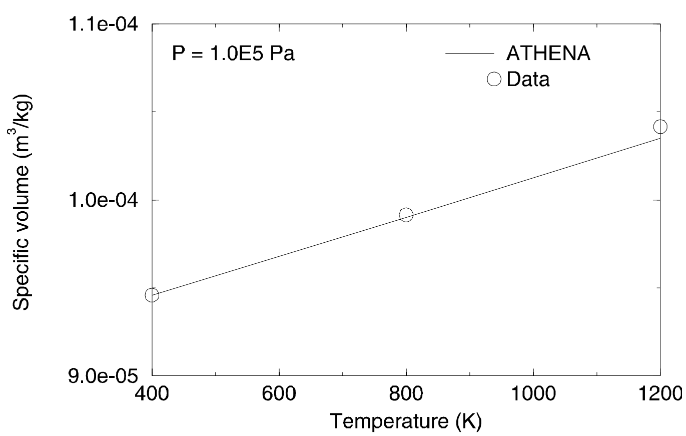

Fig. 3. Specific volume of liquid lead-bismuth versus temperature.

ATHENA uses a simplified Clausis-Clapeyron formulation for the saturation pressure, P_{sat}:

$$P_{sat} = ce^{\gamma/T} \quad (3)$$

where T is the temperature and c and γ are constants that were obtained from a least-squares curve fit of data (Nesmeyanov, 1963) and were computed to be 8.530709E9 and –2.005E4, respectively. The results of the model are compared with data in Fig. 4.

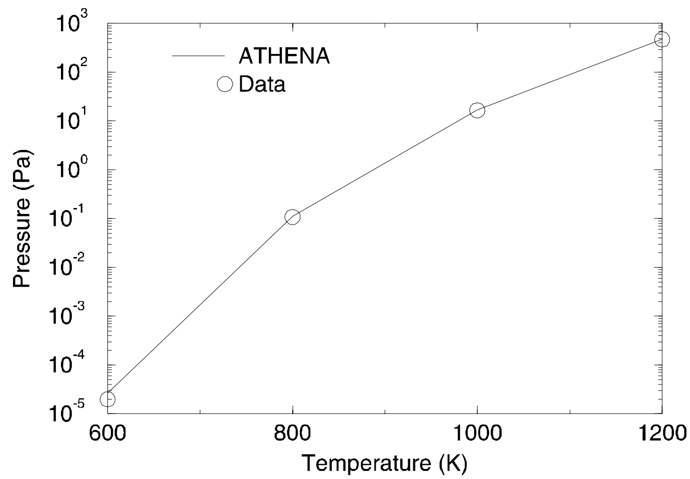

Fig. 4. Saturation pressure of lead-bismuth versus temperature.

ATHENA also requires equations for surface tension and the transport properties of dynamic viscosity and thermal conductivity. The surface tension, σ, is calculated based on data (Lyon, 1952) as:

$$\sigma = -5.5\text{x}10^{-5} (T – 1073.15) + 0.367 \quad (4)$$

where T is the temperature in degrees Kelvin. The dynamic viscosity, μ, is calculated as:

$$\mu = \nu \rho \quad (5)$$

where ν is the kinematic viscosity and ρ is the density. The kinematic viscosity and density have been correlated (Touloukian et al., 1970) as:

$$\nu = 61.423 (T - 273.15)^{-0.61106} * 10^{-7} \quad (6)$$

and

$$\rho = 10728.0 – 1.2159 (T - 273.15) \quad (7)$$

The thermal conductivity, k, is calculated as a piecewise linear function (Touloukian et al., 1970):

$$k = 9.408 - 0.00318(T-437.321) \text{ if } T<437.321 \text{ K} \quad (8)$$
$$= 9.78 + 0.00973(T-475.554) \text{ if } 437.321 \text{ K}<T<475.554 \text{ K}$$
$$= 9.78 + 0.0131(T-475.554) \text{ if } T>475.554 \text{ K}$$

ATHENA APPLICABILITY EVALUATION

The ATHENA code is based on the RELAP5 series of codes, which were developed for the thermal-hydraulic analysis of light water reactor systems. Thus, it is appropriate to question the applicability of ATHENA for the analysis of lead-bismuth cooled reactors. Consequently, a code applicability evaluation was conducted. This evaluation determined the important models and correlations for simulating lead-bismuth cooled reactors, the applicability of those models and correlations, and where necessary, additional correlations that needed to be added to the code.

One of the advantages of lead-bismuth coolant is its extremely high boiling point (2000 K). Boiling of the lead-bismuth is not of concern during normal operation and during credible transients because of the wide margin between the boiling temperature and the maximum coolant temperature at normal operation (less than 850 K). Furthermore, the fuel and cladding will melt at lower temperatures than the lead-bismuth will boil. Thus, the lead-bismuth is expected to remain single-phase within the pool. This greatly simplified the applicability evaluation since ATHENA's two-phase models, which constitute much of the coding, are relatively unimportant. The most important phenomena that the code needs to be able to simulate in the lead-bismuth coolant were judged to be single-phase wall heat transfer and friction. However, the code also needs to be able to predict the void fraction due to the injection of an inert gas and/or liquid water into the riser or due to a steam generator tube rupture because the void fraction affects the hydrostatic head and the natural circulation flow rate. Thus, the code's interphase drag model is also important for these special cases.

The applicability evaluation also recognized that phenomena that are not important in light water reactors, and thus were justifiably neglected in the RELAP5 series of codes, could be more important in reactors cooled by liquid metals. Two such phenomena, axial heat conduction in the fluid and thermal entry length, were evaluated to determine their potential importance in a reactor cooled by lead-bismuth. Finally, a fundamental limitation of ATHENA was recognized for modeling cases in which water enters the primary coolant system, such as in the reactor with the direct steam cycle or in an accident caused by the rupture of a steam generator tube.

Wall Heat Transfer

ATHENA contains many heat transfer correlations to simulate various heat transfer regimes, including forced and natural convection, nucleate boiling, transition boiling, film boiling, and condensation. However, forced convection is the only regime expected to occur on the primary side of a reactor cooled by lead-bismuth. For lead-bismuth and other liquid metals, the code calculates the forced convection Nusselt number, Nu, as:

$$Nu = 5 + 0.025\, Pe^{0.8} \quad (9)$$

where Pe is the Peclet number. This correlation is applicable for fully developed flow of a liquid metal in a tube with constant wall temperature (Bird et al., 1960). A separate correlation for natural convection is not required because the Nusselt number approaches five, rather than zero, as the Peclet number goes to zero.

ATHENA allows the user to apply correlations developed for rod bundles rather than tubes for specific heat structures. However, this option was not available for liquid metals in the original code. Thus, a correlation developed by Kazimi and Carelli (1976) for a rod bundle was added to the code. The correlation is:

$$Nu = 4.0 + 0.33(P/D)^{3.8}(Pe/100)^{0.86} + 0.16(P/D)^{5} \quad (10)$$

where P/D is the pitch-to-diameter ratio of the rods. The correlation was developed for a range of $1.1 < P/D < 1.4$ and $10 < Pe < 5000$. Kazimi and Carelli (1976) assessed the correlation using several sets of experiments that were conducted in sodium, mercury, and sodium-potassium. Most of the experiments were conducted using bare rod bundles, but a few used wire-wrapped rods. The correlation was reported to be in good agreement with the experimental data for $1.1 < P/D < 1.2$, but to under-predict Nusselt numbers when the P/D exceeded 1.2.

Wall Friction

ATHENA calculates single-phase wall friction using the Darcy-Weisbach friction factor for laminar and turbulent flow. Turbulent flow is of most interest for lead-bismuth reactors. For turbulent flow, the code uses the Zigrang-Sylvester (1985) approximation to the Colebrook-White (1939) correlation to compute the friction factor. The Zigrang-Sylvester approximation is accurate to within 0.5% of the Colebrook-White correlation (the RELAP5 Development Team, 1995). The SSC code (Guppy et al., 1983), which was developed for analysis of liquid metal fast breeder reactors, used an explicit approximation to the Colebrook-White correlation that was accurate to within 5%. The Colebrook-White correlation also is in good agreement with a correlation used in previous analyses (Greenspan et al., 1998) of lead cooled reactors. Thus, it is judged that the code's model is applicable for the calculation of single-phase wall friction in reactors cooled by lead-bismuth.

Interphase Drag

The RELAP5 series of codes has been extensively used and assessed for the thermal-hydraulic analysis of light water reactors. However, the ATHENA code has not been assessed as thoroughly for non-aqueous fluids. Consequently, the capability of the ATHENA code to predict the void fraction of a mixture of lead-bismuth and steam for vertical upflow was assessed using the El-Boher and Lesin (1988) void correlation. This correlation was developed for co-current upflow of different mixtures, including water and air, mercury and steam, and lead-bismuth and steam. The lead-bismuth/steam data were taken in a pipe that was 0.203 m in diameter and 7.5 m long. The nominal pressure and temperature were 3.5 x 10^5 Pa and 443 K, respectively. The superficial velocity of the liquid lead-bismuth varied from 0.6 to 1.6 m/s. The ratio of gas superficial velocity to liquid superficial velocity varied from about 0.35 to 5.8. The average flow quality was about 1×10^{-4}.

The El-Boher and Lesin correlation is:

$$\alpha = 1/[1+0.27(Q_R)^{-0.69}(Fr)^{-0.177}(\mu_f/\mu_g)^{0.378}(Re/We)^{0.067}] \quad (11)$$

where α is the gas volume fraction, Q_R is the volumetric flow ratio, Fr is the Froude number, μ_f/μ_g is the dynamic viscosity ratio, Re is the Reynolds number, We is the Weber number, and the subscripts f and g refer to the liquid and gas, respectively. The non-dimensional numbers are calculated as

$$Q_R = x\rho_f/[(1-x)\rho_g] = j_g/j_f \quad (12)$$

$$Fr = j_f^2/(gD) \quad (13)$$

$$Re = \rho_f j_f D/\mu_f \quad (14)$$

$$We = j_f^2 \rho_f D/\sigma_f \quad (15)$$

where

x = flow quality
ρ = density
j = superficial velocity
D = pipe diameter
g = acceleration due to gravity
σ= surface tension

Equation (11) predicted the lead-bismuth/steam data with a root-mean-square error of 10.87%.

Figure 5 compares calculated results from the default model in ATHENA with the El-Boher and Lesin correlation. The trends calculated by ATHENA were in reasonable agreement with Eq. (11). However, the calculated void fractions exceeded the values from the correlation by up to 30%.

ATHENA calculates phase slip using interphase drag coefficients. The code uses a drift flux approach for the bubbly and slug flow regimes in vertical components and converts the essential results from a drift flux correlation to an equivalent interphase drag coefficient. ATHENA used the Kataoka and Ishii (1987) drift flux correlation to calculate the results shown in Fig. 5. Slightly worse results were obtained using the other drift flux correlations that are available in the code. Consequently, the El-Boher and Lesin correlation was implemented into a modified version of ATHENA. Calculations from the modified version of the code were in excellent agreement with the correlation as shown in Fig. 6. The figure shows that the El-Boher and Lesin correlation was implemented correctly into ATHENA. Details of the implementation are provided in another paper that has not yet been published.

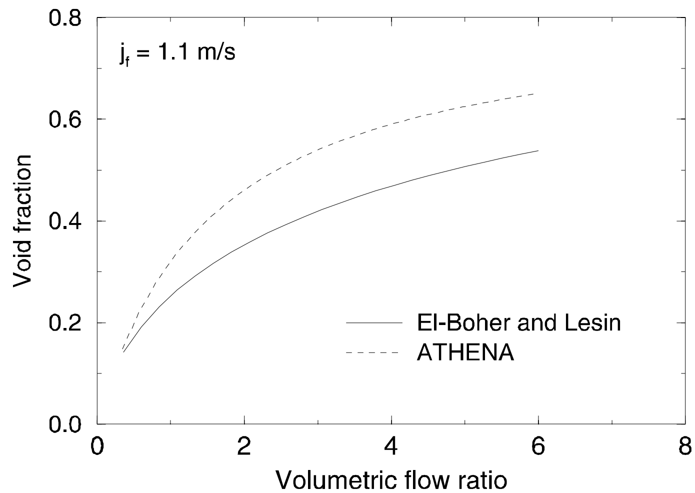

Fig. 5. A comparison of the El-Boher and Lesin correlation with ATHENA.

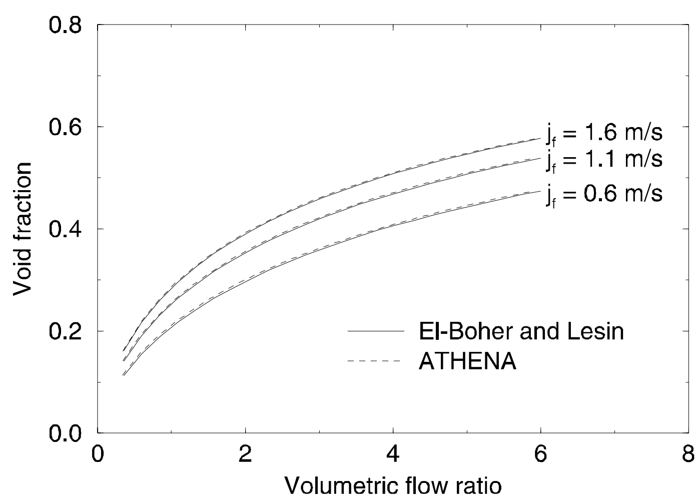

Fig. 6. A comparison of the El-Boher and Lesin correlation with the modified ATHENA code.

Axial Fluid Conduction

The thermal-conductivity in lead-bismuth is more than an order of magnitude greater than that of water. Thus, axial conduction within the fluid has the potential to be more important in lead-bismuth than in water. Axial conduction effects can generally be neglected if the Peclet number is greater than 100 (Kays and Crawford, 1980). At normal operation, the core and heat exchanger in the current forced convection design have Peclet numbers greater than 3000. The effects of axial conduction thus could begin to become significant only at very low flow rates, such as might occur during transients with a transition from forced circulation to natural circulation. The Peclet number should be checked after such transients are simulated to determine if the axial conduction in the fluid could be important. Until then, it seems appropriate to neglect axial conduction in ATHENA.

Thermal Entry Effects

The forced convection heat transfer correlations used by the code are based on fully developed flow. The thermal entry length depends on the Prandtl number, and is longer for fluids with low Prandtl number fluids, such as liquid metals, than for water. Based on results for a circular tube with constant heat flux (Kays and Crawford, 1980), the average heat transfer coefficient over the length of the core described by Buongiorno et al. (1999a) is about 25% greater than the fully developed heat transfer coefficient. The average heat transfer coefficient for the steam generator tubes is less than 10% greater than the fully developed value. Since ATHENA does not model thermal entry effects, it is expected to provide somewhat conservative calculations of fuel temperature and heat exchanger efficiency.

Limitation

The applicability evaluation determined that ATHENA has a fundamental limitation for cases in which water enters the reactor system, such as would occur in the design with a direct steam cycle or in the case of a steam generator tube rupture. The limitation arises because the code solves continuity, energy, and momentum equations for two phases of a single fluid, lead-bismuth in this case. If water enters the system, four phases could be present: liquid lead-bismuth, a tiny amount of lead-bismuth vapor, liquid water, and steam. The code cannot handle this situation mechanistically as it represents only two fluid fields, one for the liquid and one for the gas. A major revision to the code would be required to model all four phases and the interactions between them.

Any water entering the system will rapidly boil to steam, which will superheat as it comes into equilibrium with the liquid lead-bismuth. Because of the large amount of superheat, the steam is not expected to condense anywhere in the reactor coolant system except in the turbine and the condenser. Since these components are not normally modeled with ATHENA, acceptable results can probably be obtained by representing the steam as an ideal, non-condensable gas. An ATHENA control system will be required to inject an appropriate amount of non-condensable gas and to remove from the lead-bismuth coolant the amount of energy needed to boil the water to steam. Although such a control system has not been yet built, it is anticipated that one can be readily developed that will provide acceptable results for design calculations.

CORROSION EXPERIMENT

The design of the INEEL corrosion experiment is illustrated in Fig. 7. The experiment contains a small vessel, approximately 10.2 cm in diameter, which is separated into three regions by a shroud. The three regions include a riser that is located inside the shroud, a downcomer that is located between the shroud and the vessel wall, and an upper plenum region located above the top of the shroud. The experiment will initially contain a pool of molten lead-bismuth with a level above the top of the shroud. An inert gas will be injected into the riser near the bottom. The gas will flow up through the riser, reducing the hydrostatic head in the riser. The difference in hydrostatic head between the riser and downcomer will then cause liquid lead to flow up through the riser, down the downcomer, and back to the riser through a gap located at the bottom of the shroud. The gas separates in the upper plenum and will be removed through the top of the vessel. The purpose of the experiment is to determine the corrosion characteristics of the vessel wall as a function of temperature and fluid velocity in the downcomer.

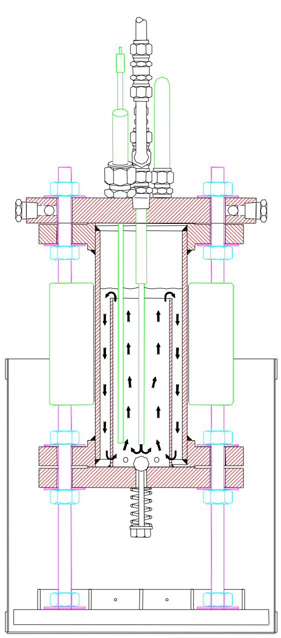

Fig. 7. Schematic of the corrosion test facility.

The corrosion experiment was modeled with ATHENA to aid in its design. Specifically, a series of calculations was performed to determine the shroud diameter that maximizes the fluid velocity in the downcomer. These calculations were performed at a pressure of $1x10^5$ Pa, a temperature of 450 C, and a gas flow rate of 0.0006 kg/s. The shroud height and thickness were assumed to be 27.9 and 0.305 cm, respectively.

The effect of the shroud inner diameter on the fluid velocity in the downcomer is presented in Fig. 8. The figure shows that the maximum downcomer fluid velocity occurred when the shroud inner diameter was about 8.1 cm. The maximum in velocity occurs because of two competing effects. The first effect is simply that due to the influence of the flow area on the fluid velocity at a constant flow rate. As the shroud diameter decreases, the downcomer flow area increases and the velocity decreases in order for the flow rate to remain constant. The second effect is that due to the influence of the downcomer hydraulic diameter and flow area on the frictional pressure drop around the flow circuit. The major hydraulic losses in the test loop are due to single-phase wall friction in the downcomer and single-phase form losses at the top and bottom of the downcomer. The hydraulic resistance of the riser, including two-phase effects, is relatively small. As the shroud diameter decreases, the downcomer flow area and hydraulic diameter increase, which decreases the frictional pressure drop across the downcomer and causes an increase in the natural circulation flow rate, which tends to increase the fluid velocity in the downcomer. Figure 8 indicates that the first effect is more important for shroud inner diameters less than 8.1 cm and that the second effect is more important at larger diameters. For example, as the inner diameter increased above 8.1 cm, the frictional pressure drop across the downcomer increased, causing the natural circulation flow rate to decrease. The effect of the smaller natural circulation flow rate more than offset the increase in velocity associated with the smaller area for a constant flow rate.

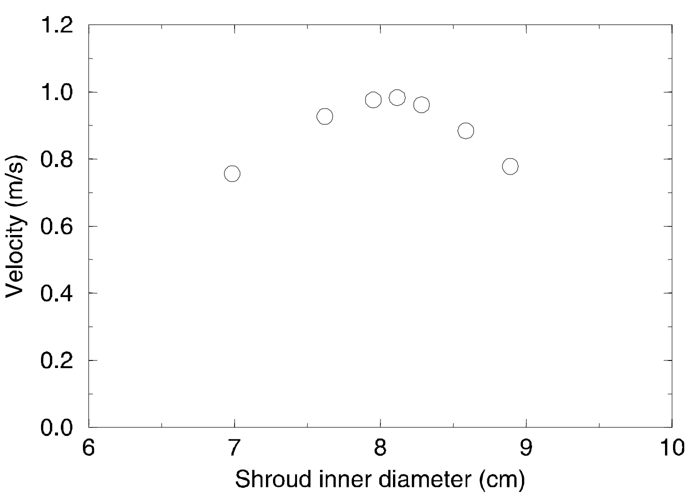

Fig. 8. Downcomer velocity versus shroud inner diameter.

Based on the results shown in Fig. 8, 3-inch schedule-10S pipe was purchased to form the inner shroud. The inner diameter of this pipe (8.28 cm) is very close to the value that maximizes the fluid velocity in the downcomer.

FUTURE ANALYTICAL WORK

The majority of the work that has been performed to date with ATHENA has been in the modification of the code for analysis of lead-bismuth cooled reactors. Only a small amount of analytical work has been actually been performed on the analysis of lead-bismuth cooled reactors. This has been limited to the development of input models describing preliminary reactor designs and the performance of full-power, steady-state calculations described by Buongiorno et al. (1999a).

The modified version of ATHENA will be used to perform design calculations and confirmatory calculations for analysis of lead-bismuth cooled reactors both at MIT and INEEL. Once the design of the reactor matures, the code will be used to determine the safety margins during various transients.

CONCLUSIONS

The ATHENA code is being used in the design and analysis of lead-bismuth cooled reactors. An evaluation was performed to determine the applicability of the code for such analysis. The evaluation showed areas where the code needed to be modified to perform its intended function. Such modifications have been performed and it is concluded that the modified code is generally applicable for analysis of lead-bismuth cooled reactors.

The most important code models relative to the analysis of lead-bismuth cooled reactors are single-phase, forced convection wall heat transfer, single-phase wall friction, and interphase drag. The existing forced convection heat transfer correlation is applicable for tubes. A correlation was added to the code to represent forced convection heat transfer in rod bundles. The existing single-phase wall friction model was judged to be applicable. The El-Boher and Lesin void correlation was added to the code to improve its capability to calculate void fraction in mixtures of lead-bismuth and steam during upflow.

The code neglects the effects of axial conduction in the fluid, but these effects were shown to be unimportant based on the current reactor design. The code will predict average heat transfer coefficients that are up to 25% lower than would be expected in the reactor because it assumes fully developed flow. This will cause the code to provide somewhat conservative predictions of fuel temperature, cladding temperature, and heat exchanger efficiency. The code cannot mechanistically represent the effects of adding water into the reactor coolant, but it is believed that the most important of these effects can be modeled adequately for design calculations.

The ATHENA code has already been used in the design of corrosion experiments that will be performed at the INEEL. The code will be also be used to perform design calculations,

calculations that confirm the existing design, and calculations to quantify the safety margins during various reactor transients.

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